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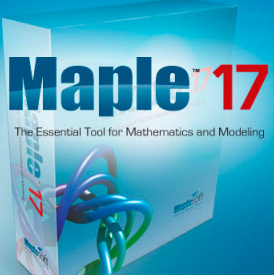
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# Variational principles for resonances. II

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Variational principles for calculating the complex poles of Green's function are given. Convergence of the numerical procedure is proved.

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## I. INTRODUCTION

This note is a continuation of Ref. 1, where the following problem was considered:

$$(-\nabla^2 - k^2)u = 0 \quad \text{in } \Omega, \quad u|_{\Gamma} = 0. \quad (1)$$

Here  $\Omega$  is an exterior domain,  $\Gamma$  is its closed smooth boundary, and  $D = \mathbb{R}^3 \setminus \Omega$  is bounded. Problem (1) has nontrivial solutions if and only if ( $\equiv$  iff)  $k$  is a complex pole  $k_q$  of the Green's function  $G(x, y, k)$  of the exterior Dirichlet problem. In Ref. 1 a stationary variational principle for resonances, i.e., complex poles  $k_q$ , was given

$$k^2 = \text{st} \{ \langle \nabla u, \nabla u \rangle / \langle u, u \rangle \}, \quad (2)$$

where st is the symbol of stationary value,

$$\langle u, v \rangle = \lim_{\epsilon \rightarrow +0} \int \exp(-\epsilon r \ln r) u(x) v(x) dx, \quad (3)$$

$$\int = \int_{\Omega}, \quad r = |x|.$$

In Ref. 1 the test functions for (2) were taken in the form

$$u_N = r^{-1} \exp(ikr) \sum_{j=0}^N \sum_{|m| \leq j} r^{-j} Y_{jm}(n) c_{jm} g(x), \quad (4)$$

where  $n = x/|x|^{-1}$ ,  $Y_{jm}$  are the spherical harmonics,  $c_{jm}$  are constants,  $k$  is a parameter, and  $g(x) \geq 0$  is a fixed smooth function vanishing on  $\Gamma$  and equal to 1 outside of some ball containing  $D$ . It was not proved in Ref. 1 that the numerical procedure suggested there converges. The question formulated in Ref. 1 concerning the justification of the numerical approach is still open. The purpose of this note is to formulate another variational principle for calculating the complex poles  $k_q$  and to prove the convergence of the numerical procedure. The method in Ref. 1 is similar to Ritz's method. The method suggested in this note is similar to Trefftz's method. The advantage of this method is that one deals with the compact operators, while in Ref. 1 the operator was not compact. Our construction is natural in the framework of the singularity and eigenmode expansion methods.<sup>2</sup> The convergence of the method will be proved. A result which is of general interest, as it seems to the author, is a construction of a stationary variational principle and a proof of convergence for a class of non-self-adjoint symmetric operators ( $B^* = \bar{B}$ ), which occur frequently in the scattering theory.

## II. A VARIATIONAL PRINCIPLE

The starting point is the following observation:  $k$  is a complex pole of  $G(x, y, k)$  iff the equation

$$Af \equiv \int_{\Gamma} g(s, t, k) f(t) dt = 0, \quad \text{Im} k < 0, \quad (5)$$

$$g(s, t, k) = \exp(ik|s-t|) / (4\pi|s-t|),$$

has a nontrivial solution. This observation and some consequences are discussed in Ref. 3. For the convenience of the reader let us note that

$$G = g - \int_{\Gamma} g(x, t, z) \frac{\partial G(t, y, z)}{\partial N_t} dt, \quad (6)$$

where  $N_t$  is the unit outer normal to  $\Gamma$  at the point  $t$ . If  $k$  is a complex pole of  $G$  of order  $r$  one can multiply (6) by  $(z-k)^r$  and take  $z \rightarrow k$  and  $x = s \in \Gamma$ . This yields Eq. (5) (see Ref. 3, pp. 290-291) with  $f \neq 0$ .

Let us formulate the following variational principle

$$F(f) \equiv |Af|_1^2 = \min, \quad \|f\| = 1, \quad (7)$$

where  $|f|_p$  is the norm in the Sobolev space  $H_p = W_2^p(\Gamma)$ ,  $\|f\| = |f|_0$ . From the above observation it follows that (7) has solutions and the min is zero if  $k = k_q$ , where  $k_q$  are the poles of  $G(x, y, k)$ . If  $k \neq k_q$  then  $\inf_{\|f\|=1} |Af|_1 > 0$ . Indeed, if there exists a sequence  $\|f_n\| = 1$ ,  $|Af_n|_1 \rightarrow 0$ , then  $f_n \rightarrow f$ ,  $\|f\| = 1$ ,  $Af = 0$ , and therefore  $k = k_q$  (see Ref. 3, p. 291). The only point which is to be explained is the convergence in  $H$ :  $f_n \rightarrow f$ . In Ref. 3 it is explained that  $A$  is a pseudo-differential operator of order  $-1$ , that is,

$$a_1 |f|_{p-1} \leq |Af|_p \leq a_2 |f|_{p-1}. \quad (8)$$

Here  $a_1, a_2 > 0$  are some constants,  $-\infty < p < \infty$  if  $\Gamma \subset C^\infty$ , and the fact that  $k \neq k_q$  was used essentially: if  $k \neq k_q$  then  $\ker A \equiv \{f: Af = 0\} = \{0\}$  and  $A$  maps  $H_p$  onto  $H_{p+1}$ . If  $|Af_n|_1 \rightarrow 0$  and  $\|f_n\| = 1$ , then (8) with  $p = 1$  shows that  $\|f_n\| \rightarrow 0$ . This contradicts the equation  $\|f_n\| = 1$ . Therefore

$$\inf_{\|f\|=1} |Af|_1 > 0 \quad \text{if } k \neq k_q. \quad (9)$$

Consider a numerical method for solving problem (7). Let  $\{f_j\}$  be a basis of  $H$ ,

$$f = f^{(n)} \equiv \sum_{j=1}^n c_j f_j. \quad (10)$$

The necessary condition for  $F(f)$  to be minimal and  $\min F(f^{(n)}) = 0$ ,  $\|f^{(n)}\| = 1$ , yields:

$$\sum_{m=1}^n a_{jm} c_m = 0 \quad 1 \leq j \leq n, \quad (11)$$

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$$a_{jm} = a_{jm}(k) = (Af_m, Af_j), \quad \sum_{j=1}^n |c_j|^2 > 0. \quad (12)$$

Thus

$$\det a_{jm}(k) = 0 \quad 1 \leq j, m \leq n. \quad (13)$$

Let  $k_q^{(n)}$  denote the roots of Eq. (13). Our first result is

**Theorem 1:** There exists  $\lim_{n \rightarrow \infty} k_q^{(n)} = k_q$ , and  $k_q$  are the poles of Green's function  $G(x, y, k)$ . Every pole  $k_q$  is a limit of a sequence  $k_q^{(n)}$ , where  $k_q^{(n)}$  are the roots of (13). Convergence is uniform in  $q$  for any finite interval  $1 \leq q \leq Q$ .

*Proof:* We will prove that: (i) Eq. (13) has roots in the circle  $|k - k_q| < \epsilon$  for any fixed  $\epsilon > 0$  however small if  $n > n(\epsilon)$  is large enough. (ii) If  $n > n(\epsilon)$  and there are no points  $k_q$  in the circle  $|k - z| < \epsilon$  then Eq. (13) has no roots in the circle  $|k - z| < \epsilon$ . An important part of the proof is the reduction of the problem to the problem with the operator  $I + T(k)$ , where  $T(k)$  is compact.

Let us fix  $\epsilon > 0$  such that in the circle  $\{k: |k - k_q| < \epsilon\} = K_\epsilon$  there are no other poles. The operator  $A = A(k)$  can be written as

$$A(k) = A_0[I + T(k)], \quad (14)$$

where

$$A_0 = A(0), \quad A_0^* = A_0 > 0 \quad \text{in } H = L^2(\Gamma),$$

$$A_0 f = \int_{\Gamma} \frac{f dt}{4\pi r_{st}}, \quad (15)$$

and

$$T(k) = A_0^{-1}[A(k) - A_0]. \quad (16)$$

The operator  $A_0$  is a bijection of  $H_p$  onto  $H_{p+1}$ ;

$$b_1 |f|_0 < |A_0 f|_1 < b_2 |f|_0, \quad b_1, b_2 = \text{const} > 0, \quad (17)$$

while  $T(k)$  is compact as a map  $H_p \rightarrow H_p$  (see Ref. 3 for details) because  $A(k) - A_0$  is an operator with a nonsingular kernel. Let us rewrite functional (7) as

$$F(f) = |A_0(I + T)f|_1^2 = \min, \quad \|f\| = 1. \quad (18)$$

From (18) and (17) it follows that the problem (7) is equivalent to

$$F_0(f) = |(I + T)f|_0^2 = \min, \quad \|f\| = 1. \quad (19)$$

The matrix of the system (11) can be written as

$$a_{jm} = ((I + T)f_m, (I + T)f_j), \quad (20)$$

where  $(\cdot, \cdot)$  denotes the scalar product which is metrically equivalent to the scalar product in  $H$ . This means that  $d_1(f, f)_0 < (f, f) < d_2(f, f)_0$ , where  $d_1 > 0$  and  $d_2$  are constants,  $f \in H$  is arbitrary. In the sequel we will not discriminate between  $(\cdot, \cdot)$  and  $(\cdot, \cdot)_0$ . This is possible because  $((I + T)f, (I + T)f)$  and  $((I + T)f, (I + T)f)_0$  attain their zero values simultaneously. The system (11) can be considered as the system which corresponds to the Ritz method for functional (19) with the test functions  $\{f_j\}$ . This completes the reduction of the original problem to the problem with the operator  $I + T(k)$ , where  $T(k)$  is a compact analytic-in- $k$  operator function on  $H$ . To prove (i) let us assume that for a fixed  $\epsilon > 0$  and  $k_q$  and all  $n$  there are no roots  $k_q^{(n)}$  of Eq. (13) in the circle  $|k - k_q| < \epsilon$ . The system (11) with the matrix (20) says that

$$((I + T)f^{(n)}, (I + T)f_j) = 0 \quad 1 \leq j \leq n, f^{(n)} \neq 0, \quad (21)$$

where

$$f^{(n)} = \sum_{j=1}^n c_j f_j. \quad (22)$$

In particular, our assumption means that

$$(\tilde{T} \equiv T + T^* + T^*T, I + \tilde{T} = (I + T^*)(I + T)),$$

$$(I + P_n \tilde{T}(k)) f^{(n)} = 0 \Rightarrow f^{(n)} \equiv 0, \quad |k - k_q| < \epsilon, \quad (23)$$

where  $P_n$  denotes the projection in  $H$  onto the linear span of  $\{f_1, \dots, f_n\}$ . Equation (23) says that  $I + P_n \tilde{T}(k)$  is invertible in the circle  $|k - k_q| < \epsilon$ . If  $n$  is large enough this implies that  $I + \tilde{T}(k)$  is invertible in the circle  $|k - k_q| < \epsilon$ , because

(\*)  $\|I + \tilde{T}(k) - (I + P_n \tilde{T}(k))\| \rightarrow 0$  as  $n \rightarrow \infty$ . This is a contradiction since  $I + \tilde{T}(k_q)$  is not invertible. Let us explain (\*).

We need to show that  $\|(I - P_n)\tilde{T}\| \rightarrow 0$  as  $n \rightarrow \infty$ . Since  $\tilde{T}(k)$  is compact it can be written as  $T_N + B_N$ , where  $\|B_N\| < d_N$ ,  $d_N \rightarrow 0$  as  $N \rightarrow \infty$ , and  $T_N$  is a finite-dimensional operator. It is sufficient to prove that  $\|(I - P_n)T_N\| \rightarrow 0$  as  $n \rightarrow \infty$ . Without loss of generality one can assume that  $T_N$  is a one-dimensional operator,  $T_N f = (f, v)u$ . Then

$$\|(I - P_n)T_N f\| = \|(I - P_n)u\| |(f, v)|$$

$$< \|f\| \|v\| \|u - P_n u\| \rightarrow 0 \quad \text{as } n \rightarrow \infty, \quad (24)$$

since  $P_n \rightarrow I$  strongly. Thus the statement (i) is proved. Note that the orthogonality of  $P_n$  is not used in (24). In order to prove (ii) we suppose that for any  $\epsilon_n > 0$ ,  $\epsilon_n \rightarrow 0$ , Eq. (13) has a root  $k^{(n)}$  in the circle  $|k - z| < \epsilon_n$  and show that under this assumption  $z$  has to be a pole of the Green's function. The assumption means that

$$[I + T(k^{(n)})] f^{(n)} = 0, \quad \|f^{(n)}\| = 1, \quad k^{(n)} \rightarrow z. \quad (25)$$

Since  $\|f^{(n)}\| = 1$ , one can extract a weakly convergent in  $H$  subsequence which is denoted again  $f^{(n)}$ ;  $f^{(n)} \rightarrow f$  ( $\rightarrow$  means weak convergence). Since  $T(k)$  is compact the sequence  $T(z)f^{(n)}$  converges strongly in  $H$ :

$$T(z)f^{(n)} \rightarrow T(z)f. \quad (26)$$

On the other hand,

$$\|T(k_n) - T(z)\| \rightarrow 0. \quad (27)$$

From (25)–(27) it follows that

$$f^{(n)} \rightarrow f, \quad \|f\| = 1, \quad (28)$$

and

$$[I + T(z)]f = 0, \quad \|f\| = 1. \quad (29)$$

The proof is complete.

### III. DISCUSSION

The variational principles (19) and (18) can be viewed as the least square method. Let us consider instead of (13) and (20) the following equation:

$$\det b_{jm}(k) = 0, \quad 1 \leq j, m \leq n, \quad b_{jm} \equiv ((I + T(k))f_m, f_j). \quad (30)$$

Arguments similar to the ones given in Ref. 3, pp. 192–193 show that: (i) For any  $\epsilon > 0$  and  $k_q$  there exists a root  $\tilde{k}_q^{(n)}$  of Eq. (30), such that  $|k_q - \tilde{k}_q^{(n)}| < \epsilon$  if  $n > n(\epsilon)$ . (ii) If  $\tilde{k}_q^{(n)}$  is a sequence of the roots of Eq. (30) and  $\tilde{k}_q^{(n)} \rightarrow k_q$  as  $n \rightarrow \infty$ , then  $k_q$  is a pole of the Green's function. Equation (30) can be viewed as a necessary condition for the linear system of the

Galerkin method for the equation  $(I + T(k))f = 0$  to have a nontrivial solution. The Galerkin equation is of the form

$$(f^{(n)} + T(k)f^{(n)}, f_j) = 0 \quad 1 \leq j \leq n, \quad (31)$$

where  $f^{(n)}$  is defined in (22). The basic idea is that the poles  $k_q$  are the points at which the operator  $I + T(k)$  is not invertible. These points can be found by the Galerkin method, by minimizing functional (19) or by some other method. It is interesting to note that the Galerkin equation (31) can be obtained also as a necessary condition for the stationary variational principle

$$((I + T(k))f, f) = \text{st}, \quad \|f\| > 0, \quad (32)$$

where st means stationary value. This is not true for an arbitrary operator, but the operator  $B \equiv I + T(k)$  is a symmetric non-self-adjoint operator on  $H = L^2(\Gamma)$ , that is

$$\overline{B^*} = B \quad \text{or} \quad B(s, t) = B(t, s) \neq \overline{B(t, s)}. \quad (33)$$

Therefore the necessary condition for (32), which can be written as

$$(Bf, h) + (Bh, f) = 0 \quad \text{for all } h \in H, \quad (34)$$

yields

$$0 = (Bf, h) + (\overline{B^*f}, \bar{h}) = (Bf, h) + (B\bar{f}, \bar{h}). \quad (35)$$

Let  $h = v$ , where  $v \in H$  is an arbitrary real-valued function.

Then (35) says that

$$0 = B(f + \bar{f}). \quad (36)$$

Let  $h = iv$ . Then (35) says that

$$0 = B(f - \bar{f}). \quad (37)$$

From (36) and (37) it follows that the equation

$$Bf = (I + T(k))f = 0, \quad \|f\| > 0 \quad (38)$$

is a necessary condition for (32).

Our aim is to show that Eq. (31) is a necessary condition for the problem

$$(Bf, f) = \text{st}, \quad \|f\| > 0. \quad (39)$$

Let us take  $f = f^{(n)}$  and rewrite (39) as

$$\sum_{j,m=1}^n b_{jm} c_m \bar{c}_j = \text{st}, \quad b_{jm} = (Bf_m, f_j). \quad (40)$$

In general assumption (33) does not imply the equality  $b_{jm} = b_{mj}$ . Therefore the following lemma is of use.

**Lemma 1:** Assume (33) and

$$f_j = \bar{f}_j, \quad j = 1, 2, \dots \quad (41)$$

Then

$$b_{jm} = b_{mj}. \quad (42)$$

The proof is immediate.

**Proposition 1:** Assume (33) and (41). Then a necessary condition for (40) is the system (31).

*Proof:* The operator  $B = I + T(k)$  satisfies (33). From this and Lemma 1, Proposition 1 follows.

**Remark 1:** The results of Sec. III give a convergent numerical scheme for a stationary variational principle (32) with a compact operator  $T$  satisfying condition (33), i.e., symmetric non-self-adjointness. Such operators occur frequently in the scattering theory. A simple example is problem (1). There are other examples in Ref. 4.

**Remark 2:** A numerical scheme for calculating the resonances based on theorem 1 is as follows: (1) Calculate matrix  $a_{jm}$  by formula (11). (2) Find roots of Eq. (13). The corresponding solutions of (1) can also be calculated by this numerical procedure: Find  $f^{(n)}$  by formula (10) and  $u^{(n)} = Af^{(n)}$  is the approximate solution of (1), which converges to the exact solution of (1) as  $n \rightarrow \infty$ . This exact solution is of the form  $u = A(k_q)f, f = \lim f^{(n)}$  as  $n \rightarrow \infty$  and lim here means the limit in  $H = L^2(\Gamma)$ .

**Remark 3:** For numerical calculations instead of principle (32) one should use the equivalent principle

$$(A(k)f, f) = \text{st}, \quad \|f\| > 0. \quad (43)$$

The equivalence of (43) and (32) follows from the fact that the necessary condition for (43) is the equation

$$A(k)f = A_0(I + T(k))f = 0, \quad \|f\| > 0, \quad (44)$$

which is equivalent to the necessary condition (38) for (32) because  $\ker A_0 = \{0\}$ . If one takes  $f = f^{(n)}$  as in (22), then the analog of (30) is

$$\det(A(k)f_m, f_j) = 0 \quad 1 \leq m, j \leq n, \quad (45)$$

and the convergence of the numerical procedure follows from the arguments given for Eq. (30).

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